Development of nuclear fuel cycle scenario code NMB4.0 for integral analysis from front to back end of nuclear fuel cycle

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Background

Future demand for nuclear power
Politics, R&D, Energy market...
➡ Upside/Maintain/Downside

Nuclear fuel cycle
✓ Policy of fuel cycle and its process conditions will be varied
✓ Fuel cycle is a system established by multiple processes
⇔ Advanced nuclear energy system was constructed by setting appropriate conditions

Strategy of Back-end
✓ Establishment of Back-end processes
✓ R&D have been progressed for multiple purposes
✓ Back-end is greatly affected by Front-end scenarios

Nuclear fuel cycle simulation required by Front & Back-end integrated approach
Comparison of nuclear fuel cycle simulation codes based on NEA Benchmark & recent progress

<table>
<thead>
<tr>
<th>Code</th>
<th>NMB4.0</th>
<th>ANICCA</th>
<th>COSI</th>
<th>FAMILY-21</th>
<th>EVOLCODE</th>
<th>VISION</th>
<th>DESAE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Institution</td>
<td>TokyoTech/JAEA</td>
<td>SCK CEN</td>
<td>CEA</td>
<td>JAEA</td>
<td>CIEMAT</td>
<td>INL</td>
<td>RKI</td>
</tr>
<tr>
<td>Treated nuclides</td>
<td>179 (26 AN 153 FP)</td>
<td>3850</td>
<td>21</td>
<td>20 AN</td>
<td>81</td>
<td>17 (15 AN 2 FP)</td>
<td></td>
</tr>
<tr>
<td>Depletion calculation model</td>
<td>Okamura explicit method</td>
<td>CRAM16</td>
<td>CESAR5.3 &amp; Matrix method</td>
<td>Matrix exponential method</td>
<td>ORIGEN2.2</td>
<td>ORIGEN2</td>
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<tr>
<td>Waste conditioning modeling</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
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<td>Repository assessment</td>
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<td>Yes</td>
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<tr>
<td>Access</td>
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<td></td>
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</tbody>
</table>

AN: Actinide, RKI: Russian Kurchatov Institute

Track many nuclides × High speed × Flexible back-end modeling × OPEN access
Main features

1. Number of nuclides (179 nuclides: 26 actinide & 153 FP)
2. Reduced calculation time of depletion calculation (Okamura explicit method)
3. Introduction of Back-end Module

Integral analysis from front to back end of nuclear fuel cycle
Selection of 153 FP nuclides for NMB4.0

<table>
<thead>
<tr>
<th>Purpose</th>
<th>Problem</th>
</tr>
</thead>
<tbody>
<tr>
<td>✓ Flexible partitioning</td>
<td>✓ Calculation speed</td>
</tr>
<tr>
<td>✓ Accurate waste property</td>
<td></td>
</tr>
</tbody>
</table>
Selection flow of 153 FP nuclides (FPs)

- ORIGEN 1200 FPs
- Depletion cal.
  - ✓ LWR-UO2
  - ✓ LWR-MOX
  - ✓ FBR

Selection
- 5 Factors
  - ✓ Mass
  - ✓ Decay heat
  - ✓ Radioactivity
  - ✓ Toxicity
  - ✓ Mo & PGM

- Half life
  \[ T_{1/2} \geq 2 \text{days} \]

- Burn-up & Decay Chain

T. OKAMURA et al., JAEA-Data/Code 2020-023, 2021

- ✓ 5 factors were considered by importance of back-end scenario
- ✓ FPs were selected to agree the calculation result of ORIGEN by more than 99.9% among the all depletion calculation & factors

- Transmittal memo of CCC371/17, ORNL, 2002
Modification of depletion calculation method

Okamura explicit methods (OEM)
Depletion calculation

- Differential equation
  \[ \frac{d}{dt} X = AX \]

- Matrix Exponential method
  \[ X(t + \Delta t) = \left( I + A\Delta t + \frac{1}{2!} (A\Delta t)^2 + \frac{1}{3!} (A\Delta t)^3 + \cdots \right) X(0) \]

✓ Every Reactor, Fuel batch... (Over 1000 times)
✓ Accurate calculation of short half-life nuclides (Including 153 FPs)
  ➡ Shorten time step or Higher order calculation (Time↑)

A method for accurately calculating short half-life nuclides at low calculation cost

⇒ Okamura explicit method (OEM)
Modification of Matrix Exponential

Matrix Exponential (1\textsuperscript{st} Order)

\[ X(t + \Delta t) = (I + A\Delta t)X(0) \]

Ex.) Nuclide \( i \) has a short half-life:
\[ A_{ii} = -\lambda_i \text{ (Large negative value)} \]
\[ 1 + A_{ii}\Delta t < 0 \text{ (Calculation fails)} \]

Corrected time step

\[ \tilde{\Delta}t_i = e^{A_{ii}\Delta t} - 1 \]
\[ \tilde{\Delta}t = \begin{pmatrix} \tilde{t}_1 & \tilde{t}_i & \tilde{t}_N \\ \vdots & \vdots & \vdots \\ \tilde{t}_i & \tilde{t}_i & \tilde{t}_N \end{pmatrix} \]

- \textbf{Okamura explicit method - 1}
\[ X(t + \Delta t) = (I + A \circ \tilde{\Delta}t)X(0) \]

- \textbf{Okamura explicit method - 2}
\[ X(t + \Delta t) = (I + A \circ \tilde{\Delta}t^T)X(0) \]

Accurate & stable calculation can be obtained even with 1\textsuperscript{st} order approximation by introducing \( \tilde{\Delta}t_i \)
Comparison of Speed & Accuracy

- Conditions: $17 \times 17$ PWR, 45 GWd/tHM, 1200 days
- PC Specs: CPU: Intel Corei9-9900K @ 3.60GHz/Memory: 32.0 GB

- Calculation failed under the time steps $<10^{-3}$ GWd. (0.8h) with MEM
- Calculation did not fail under the longer time step with OEM
- The difference did not widen until time step 1 GWd. (32 days)
- At 10 GWd., the update step of the cross-section library was larger than that of ORIGEN, and the accuracy was reduced by about 2%.
- About 200 times accelerated by the OEM (comparison between 0.001 and 1 GWd.)

Depletion cal. 6000 Times... 13-14 h $\implies 5$ min
Back-end Module in NMB4.0
Back-end module

Flexibility
✓ Partitioning (MA, Sr, Cs...)
✓ Stabilization methods
✓ Storage period
✓ Geological repository layout etc.
WM conditions can be set for individual waste

Comprehensive WM Output
✓ Waste amount & Foot-print
✓ Nuclide composition
✓ Limiting factor for determining WM scenario
✓ Radioactivity, Decay heat, Toxicity
✓ Nuclide migration after disposal etc.

NMB4.0 was developed for the flexible and comprehensive analysis of back-end simulation
Benchmark

Based on the Japan’s geological disposal program

vs Static NFC simulation
ORIGEN + COMSOL

Scenario
PWR-UO2 ➔ 4-yr cooling ➔ PUREX ➔ Vitrification ➔ 50-yr Storage ➔ Disposal

Calculated amount
① Waste amount
② Decay Heat
③ Radioactivity
④ Mo content
⑤ PGM content
⑥ Buffer temperature

Heat transfer calculation for design of geological repository
★ Under prepared model data base
○ The layout, occupied area...
× Physical data, disposal depth...

Model of geological repository
Buffer temperature = $T_B$ (°C)
Comparison of benchmark calculation results in ORIGEN+COMSOL & NMB4.0 (PWR, 45 GWd/tHM, 4-year cooling of SF, PUREX, 44.4 m²)

<table>
<thead>
<tr>
<th>Amounts</th>
<th>Code</th>
<th>ORIGEN+COMSOL ①</th>
<th>NMB4.0 ②</th>
<th>(②/① - 1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number, unit/tHM</td>
<td></td>
<td>1.24</td>
<td>1.23</td>
<td>-0.528%</td>
</tr>
<tr>
<td>Decay Heat (Initial), kW/unit</td>
<td></td>
<td>2.39</td>
<td>2.39</td>
<td>-0.271%</td>
</tr>
<tr>
<td>Decay Heat (Disposal), kW/unit</td>
<td></td>
<td>0.347</td>
<td>0.347</td>
<td>0.0362%</td>
</tr>
<tr>
<td>Radioactivity (Initial), Bq/unit</td>
<td></td>
<td>2.29E+16</td>
<td>2.3E+16</td>
<td>0.0925%</td>
</tr>
<tr>
<td>Radioactivity (Disposal), Bq/unit</td>
<td></td>
<td>4.08E+15</td>
<td>4.09E+15</td>
<td>0.194%</td>
</tr>
<tr>
<td>Mo content, wt%</td>
<td></td>
<td>1.39%</td>
<td>1.38%</td>
<td>0.185%</td>
</tr>
<tr>
<td>PGM content, wt%</td>
<td></td>
<td>1.42%</td>
<td>1.42%</td>
<td>0.129%</td>
</tr>
<tr>
<td>Max Buffer temp., °C</td>
<td></td>
<td>97.8</td>
<td>97.8</td>
<td>0.0117%</td>
</tr>
</tbody>
</table>

The calculation accuracy of NMB4.0 is equivalent to that of ORIGEN
NEA Benchmark study
NEA benchmark in 2012 vs Dynamic NFC Codes

- FAMILY21 (JAEA)
- COSI6 (CEA)
- EVOLCODE (CIEMAT (Spain))
- VISION (INL)
- DESAE (Russian Research Centre)
- ANICCA (SCK • CEN)

**Scenarios**

S1: PWR-UO2
S2: PWR-UO2+PWR-MOX
S3: PWR-UO2+PWR-MOX+FBR

**Calculated amount**

Fuel fabrication needs, Irradiated fuel inventory, Reprocessing mass flow, TRU loss etc.
Result (S1)

Scenario 1

Natural Uranium needs

Enriched Uranium needs

LWR UOX Irradiated fuel inventory

Scenario 1

Generation scenario

- Natural Uranium needs
- Enriched Uranium needs
- LWR UOX Irradiated fuel inventory
MOX fabrication needs

Pu for fabrication

Pu loss
Result (S3)

Scenario 3

FR MOX + axial blanket fabrication

FR MOX+ Axial blanket Irradiated fuel inventory

Pu loss

Generation scenario
Developed **NMB4.0**

- The selected 179 nuclides are tracked
- Okamura explicit method was invented for faster & stabilized depletion calculation
  - Correct $\Delta t$ of matrix exponential with $\Delta t_i$
  - Stabilized calculation even if the diagonal component takes a large negative value
- Developed back-end module for flexible WM simulation

**Integrated analysis of nuclear fuel cycle simulation**

**Next steps**

- Implement the Indexes related to NFC such as Economics, Environmental impact & Risk etc.
- Publish NMB4.0 as the open code
Thank you for your attention

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- Some of results were based on joint research program between JAEA and TokyoTech
- We are grateful to Dr. Ivan MERINO for supporting